

=> fil reg
FILE 'REGISTRY' ENTERED AT 18:13:45 ON 11 FEB 2003
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 10 FEB 2003 HIGHEST RN 488699-93-0
DICTIONARY FILE UPDATES: 10 FEB 2003 HIGHEST RN 488699-93-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> d sta que 146

L10 STR

8

O

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N~~C-X~C~~N~~C—C
1 2 3 4 5 6

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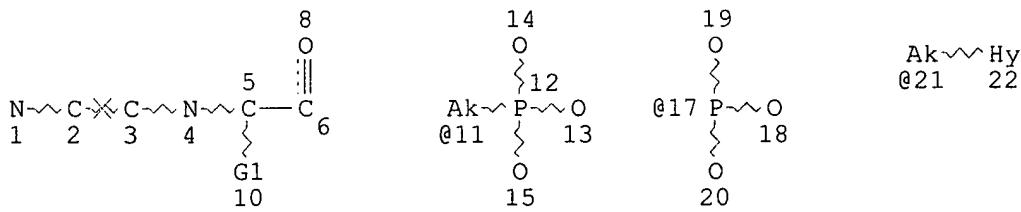
NSPEC IS RC AT 2
NSPEC IS RC AT 3
NSPEC IS RC AT 5
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 7

STEREO ATTRIBUTES: NONE

L11 SCR 2016 OR 1932
L13 12905 SEA FILE=REGISTRY SSS FUL L10 AND L11
L14 STR



Hy @24

VAR G1=17/11/24/21
NODE ATTRIBUTES:

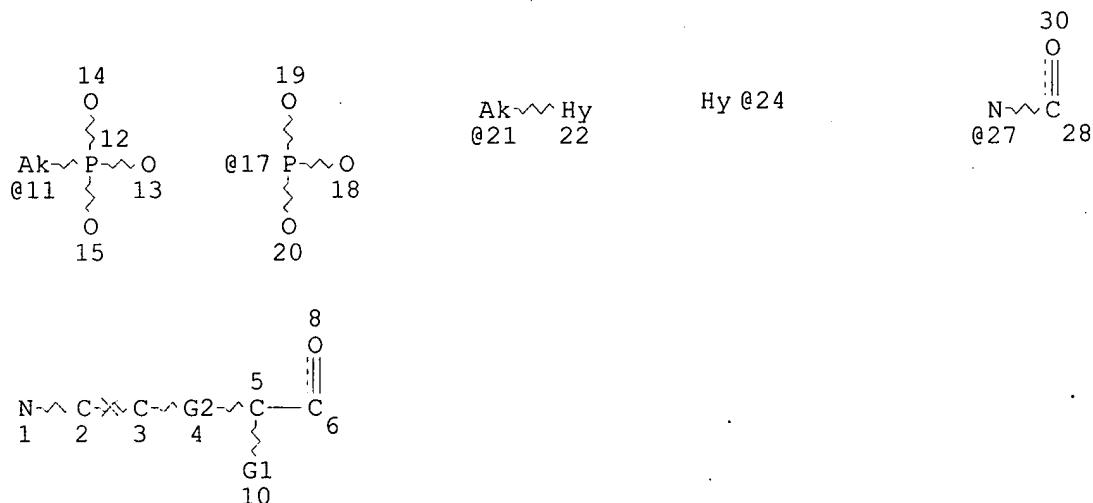
NSPEC IS RC AT 2
 NSPEC IS RC AT 3
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 DEFAULT MLEVEL IS ATOM
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 ECOUNT IS M1 B AT 22
 ECOUNT IS M1 B AT 24

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RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

L16 272 SEA FILE=REGISTRY SUB=L13 SSS FUL L14
 L44 STR



VAR G1=17/11/24/21

VAR G2=NH/27

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NSPEC IS RC AT 2
 NSPEC IS RC AT 3
 NSPEC IS RC AT 5
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED
 ECOUNT IS M1 B AT 22
 ECOUNT IS M1 B AT 24

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE

L46 266 SEA FILE=REGISTRY SUB=L16 SSS FUL L44

100.0% PROCESSED 272 ITERATIONS
 SEARCH TIME: 00.00.01

266 ANSWERS

> d his

(FILE 'HOME' ENTERED AT 17:23:08 ON 11 FEB 2003)
 SET COST OFF

FILE 'HCAPLUS' ENTERED AT 17:23:19 ON 11 FEB 2003
 E WO2000-EP1852/AP, PRN

L1 1 S E3,E4
 E DE99-19909373/AP, PRN
 L2 1 S E3,E4
 L3 1 S L1,L2
 E BOCK H/AU
 L4 284 S E3-E14
 E BOCK HOLGER/AU
 L5 5 S E3
 E LINDHORST T/AU
 L6 7 S E3,E4,E8
 E UGICHEM/AP,CS
 E UGICHEM/PA,CS
 L7 1 S E3-E6
 L8 1 S L3 AND L4-L7
 SEL RN

FILE 'REGISTRY' ENTERED AT 17:25:18 ON 11 FEB 2003

L9 19 S E1-E19
 L10 STR
 L11 SCR 2016 OR 1932
 L12 50 S L10 AND L11 SAM
 L13 12905 S L10 AND L11 FUL
 SAV TEMP L13 YOU914052/A
 L14 STR L10
 L15 9 S L14 SAM SUB=L13
 L16 272 S L14 FUL SUB=L13
 SAV L16 YOU914052A/A
 L17 9 S L9 AND B/ELS
 L18 58 S L16 AND 1062/RID
 L19 12 S L16 AND B/ELS NOT L18
 L20 6 S L19 NOT BOC2O-C6/ES
 L21 64 S L18,L20
 L22 205 S L16 AND P/ELS
 L23 3 S L21 AND L22
 L24 11 S L9 AND L13
 L25 8 S L9 NOT L24
 L26 67 S L21,L24
 L27 199 S L22 NOT L26

FILE 'HCAPLUS' ENTERED AT 17:41:56 ON 11 FEB 2003

E PEPTIDE NUCLEIC ACID/CT
 E E4+ALL

L28 1626 S E3
 L29 4958 S E4-E6/BI
 L30 2196 S PEPTIDE NUCLEIC ACID
 L31 5931 S L28-L30
 L32 26 S L26
 L33 67 S L27
 L34 1 S L31 AND L32,L33
 L35 1 S L4-L7 AND L32,L33
 L36 1 S L8,L34,L35
 L37 91 S L32,L33 AND (PD<=20000303 OR PRD<=20000303 OR AD<=20000303)
 L38 14 S L37 AND P/DT
 L39 13 S L38 NOT L36
 SEL HIT RN

FILE 'REGISTRY' ENTERED AT 17:45:12 ON 11 FEB 2003

L40 60 S E1-E60
 L41 4 S L40 AND B/ELS
 L42 STR L14
 L43 0 S L42 SAM SUB=L16

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L44      STR L42
L45      8 S L44 SAM SUB=L16
L46      266 S L44 FUL SUB=L16
          SAV L46 YOU914052B/A
L47      66 S L46 AND B/ELS
L48      6 S L47 NOT L26
L49      60 S L47 NOT L48
L50      7 S L26 NOT L49
L51      4 S L50 AND B/ELS
L52      64 S L49,L51
L53      33 S L52 AND SQL/FA
L54      31 S L52 NOT L53
L55      8 S L54 AND NCNC3/ES
L56      56 S L52 NOT L55
L57      197 S L46 NOT L47-L56
L58      199 S L27,L57
L59      74 S L58 AND SQL/FA
L60      125 S L58 NOT L59
L61      255 S L21,L27 NOT L24
L62      56 S L61 AND B/ELS
L63      23 S L62 NOT SQL/FA
L64      199 S L61 AND P/ELS
L65      125 S L64 NOT SQL/FA
L66      116 S L65 AND 1/NC

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FILE 'HCAPLUS' ENTERED AT 18:04:26 ON 11 FEB 2003

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L67      1 S L24
L68      8 S L32,L33 AND ?OLIGO?
L69      21 S L32,L33 AND 29/SC,SX
L70      2 S L32,L33 (L) POLYM?
          E RADIOTHERAPY/CT
L71      2318 S E4,E13,E14
          E E3+ALL
L72      13368 S E6+NT
L73      3 S L32,L33 AND L71,L72
L74      4 S L36,L67,L70,L73
L75      1 S L68 AND L74
L76      7 S L68 NOT L74
L77      4 S L76 NOT RHIZOCTICIN?
          SEL DN AN 2
L78      1 S L77 AND E1-E3
L79      5 S L74,L75,L78
L80      4 S L79 NOT NONHYDRO?/TI
L81      13 S L39 NOT L80
          SEL DN AN 8
L82      1 S E4-E6
L83      5 S L80,L82

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FILE 'REGISTRY' ENTERED AT 18:12:10 ON 11 FEB 2003

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FILE 'HCAPLUS' ENTERED AT 18:12:26 ON 11 FEB 2003
L84      5 S L83 AND L32,L33

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FILE 'REGISTRY' ENTERED AT 18:13:45 ON 11 FEB 2003

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=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 18:13:56 ON 11 FEB 2003
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FILE COVERS 1907 - 11 Feb 2003 VOL 138 ISS 7
 FILE LAST UPDATED: 10 Feb 2003 (20030210/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d 183 all hitstr tot

L83 ANSWER 1 OF 5 HCPLUS COPYRIGHT 2003 ACS
 AN 2000:628164 HCPLUS
 DN 133:177496
 TI Preparation of substituted monomers for synthesis of PNAs contg. carborane or phosphate side-chains for use in cancer therapy
 IN Bock, Holger; Lindhorst, Thomas
 PA UgiChem GmbH, Germany
 SO PCT Int. Appl., 30 pp.
 CODEN: PIXXD2
 DT Patent
 LA German
 IC ICM C07K014-00
 ICS C07K005-06
 CC 34-3 (Amino Acids, Peptides, and Proteins)
 Section cross-reference(s): 1, 29, 33
 FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|--|------------|--------------|------------------|--------------|
| PI | WO 2000052038 | A1 | 20000908 | WO 2000-EP1852 | 20000303 <-- |
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| | DE 19909373 | A1 | 20001005 | DE 1999-19909373 | 19990303 <-- |
| | EP 1157031 | A1 | 20011128 | EP 2000-912543 | 20000303 <-- |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| | JP 2002541068 | T2 | 20021203 | JP 2000-602262 | 20000303 <-- |
| PRAI | DE 1999-19909373 | A | 19990303 <-- | | |
| | WO 2000-EP1852 | W | 20000303 <-- | | |
| OS | MARPAT | 133:177496 | | | |
| GI | | | | | |

present application

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to novel oligomers, contg. PNA units substituted by phosphonic acid ester, phosphonic acid or carborane

functions, and the **PNA** monomers from which the novel **oligomers** are produced, for use in cancer therapy as boron neutron capture agents (no data). Thus, N4-benzyloxycarbonylcytocinyl acetic acid, 1,2-dicarbadodecaborane(12)-1-acetaldehyde, N-butoxycarbonyl ethylenediamine, and 2-isocyano-2,2-(dimethyl)ethyl carboxylic acid Ph ester were reacted to give (I; R = (CH₃)₃COC(O); R₁ = PhCH₂OC(O); R₂ = C₂B₁₀H₁₀; R₃ = OH); similarly prep'd. were I, R, R₁, R₃ as given; R₂ = P(O)(OEt)₂ (II) and I, R, R₁ as given, R₂ = C₂B₁₀H₁₀; R₃ = polymer support (III). Using an automated synthesis routine, and monomers I, II, and III, trimer IV was synthesized.

ST carborane monomer prepn **PNA** cancer radiotherapy boron neutron capture

IT **Radiotherapy**

(boron-neutron capture; prep'n. of

· substituted monomers for synthesis of **PNA**s contg. carborane side-chains for use in cancer therapy)

IT Antitumor agents

(prep'n. of substituted monomers for synthesis of **PNA**s contg. carborane side-chains for use in cancer therapy)

IT Carboranes

RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prep'n. of substituted monomers for synthesis of **PNA**s contg. carborane side-chains for use in cancer therapy)

IT **Peptide nucleic acids**

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prep'n. of substituted monomers for synthesis of **PNA**s contg. carborane side-chains for use in cancer therapy)

IT **288582-19-4P**

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prep'n. of substituted monomers for synthesis of **PNA**s contg. carborane or phosphate side-chains for use in cancer therapy)

IT 1606-75-3 20394-09-6 20924-05-4 57260-73-8 144564-95-4

234772-37-3 288582-09-2D, polymer-bound 288582-12-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(prep'n. of substituted monomers for synthesis of **PNA**s contg. carborane side-chains for use in cancer therapy)

IT **288582-07-0P 288582-10-5DP, polymer-bound**

288582-11-6DP, polymer-bound 288582-11-6P

288582-13-8P 288582-14-9P 288582-15-0P

288582-17-2DP, polymer-bound 288582-18-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prep'n. of substituted monomers for synthesis of **PNA**s contg. carborane side-chains for use in cancer therapy)

IT **288582-08-1P 288582-16-1P**

RL: SPN (Synthetic preparation); PREP (Preparation)

(prep'n. of substituted monomers for synthesis of **PNA**s contg. carborane side-chains for use in cancer therapy)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Bayer Ag; DE 19640974 A 1998 HCPLUS

(2) Hoechst Ag; DE 19508923 A 1996 HCPLUS

IT **288582-19-4P**

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

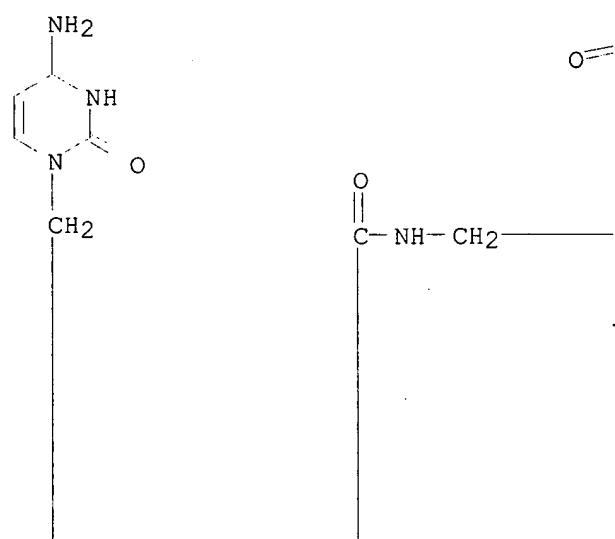
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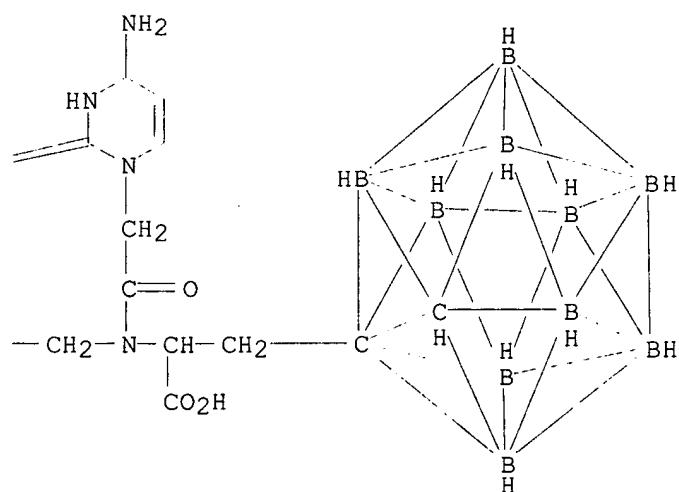
CN 3,6,9,12,15-Pentaazaheptadecanoic acid, 17-amino-3,9,15-tris[(4-amino-3,4-

dihydro-2-oxo-1(2H)-pyrimidinyl)acetyl]-2,14-bis(1,2-dicarbadodecaboran(12)-1-ylmethyl)-12-[(diethoxyphosphinyl)methyl]-7,13-dioxo- (9CI) (CA INDEX NAME)

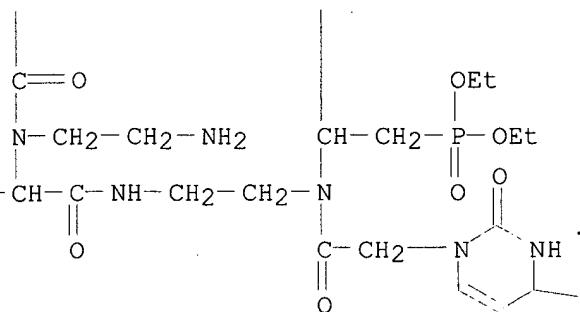
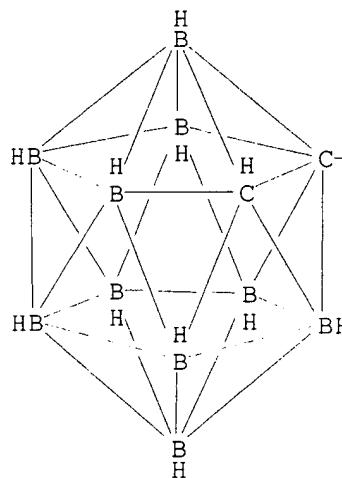
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PAGE 1-B



PAGE 2-A

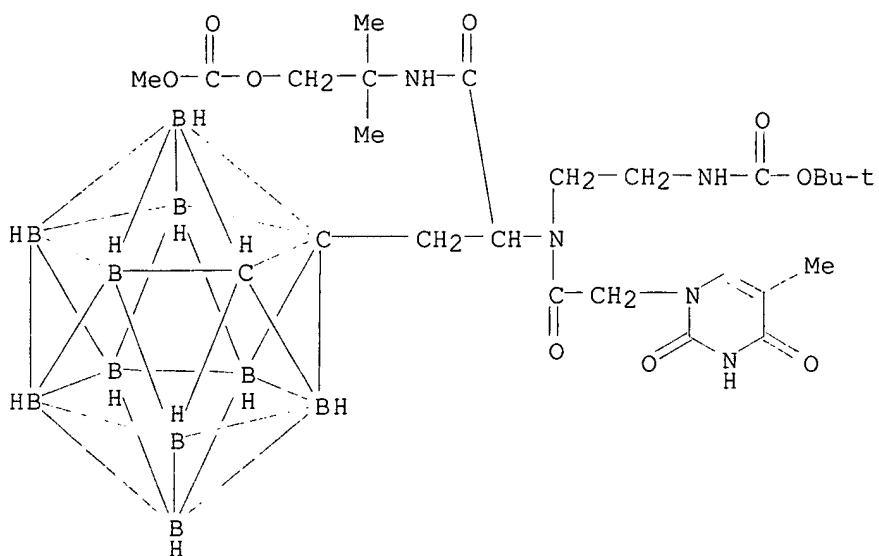


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NH₂

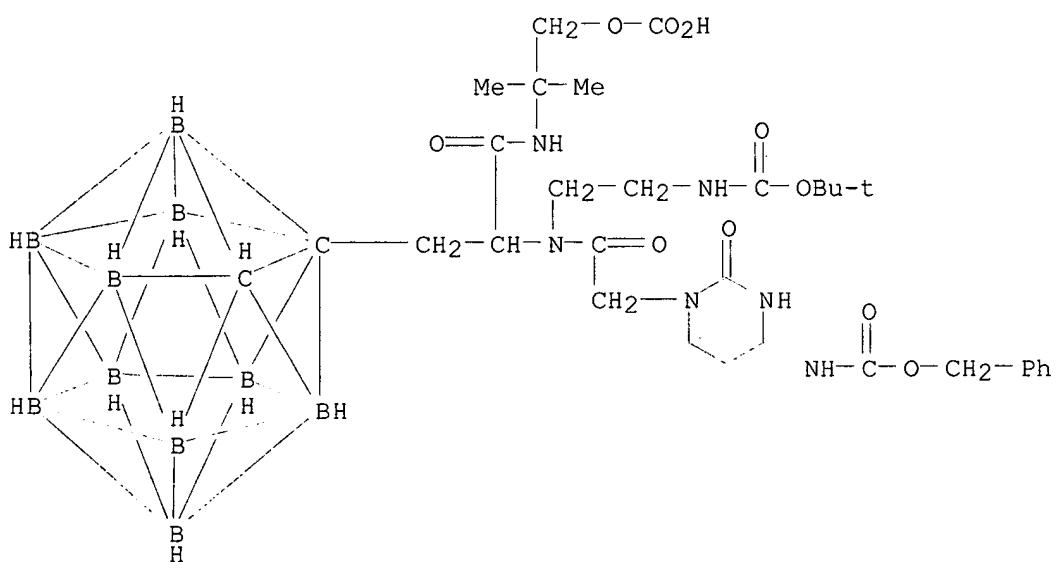
IT 288582-07-0P 288582-10-5DP, polymer-bound
 288582-11-6DP, polymer-bound 288582-11-6P
 288582-13-8P 288582-14-9P 288582-15-0P
 288582-17-2DP, polymer-bound 288582-18-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. of substituted monomers for synthesis of PNAs contg.
 carborane side-chains for use in cancer therapy)

RN 288582-07-0 HCPLUS
 CN 2-Oxa-5,8,11-triazadodecanedioic acid, 7-(1,2-dicarbadodecaboran(12)-1-ylmethyl)-8-[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-4,4-dimethyl-6-oxo-, 12-(1,1-dimethylethyl) 1-methyl ester (9CI) (CA INDEX NAME)



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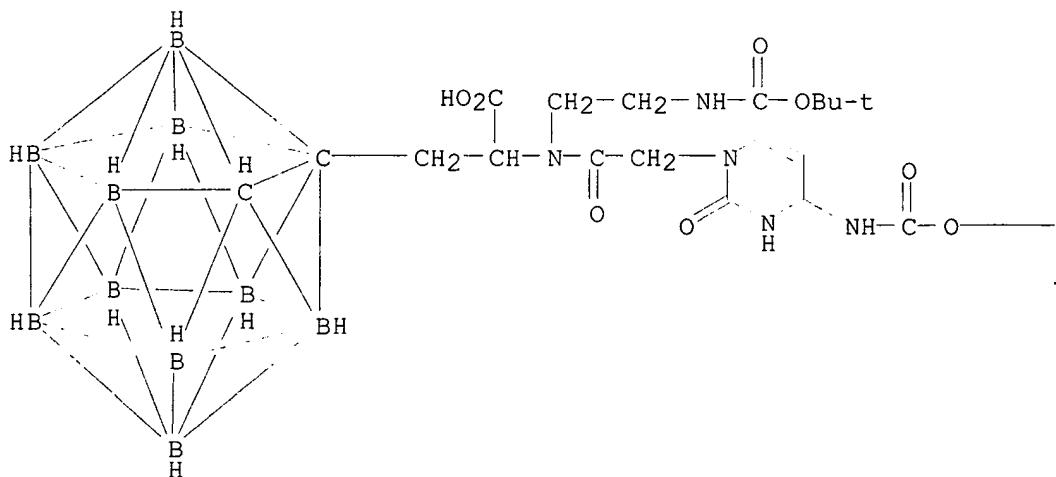
CN 2-Oxa-5,8,11-triazadodecanedioic acid, 7-(1,2-dicarbadodecaboran(12)-1-ylmethyl)-8-[3,4-dihydro-2-oxo-4-[(phenylmethoxy)carbonyl]amino]-1(2H)-pyrimidinyl]acetyl]-4,4-dimethyl-6-oxo-, 12-(1,1-dimethylethyl) ester
(9CI) (CA INDEX NAME)



RN 288582-11-6 HCAPLUS

CN 1,2-Dicarbadodecaborane(12)-1-propanoic acid, .alpha.-[[3,4-dihydro-2-oxo-4-[(phenylmethoxy)carbonyl]amino]-1(2H)-pyrimidinyl]acetyl][2-[(1,1-dimethylethoxy)carbonyl]amino]ethyl]amino]- (9CI) (CA INDEX NAME)

PAGE 1-A

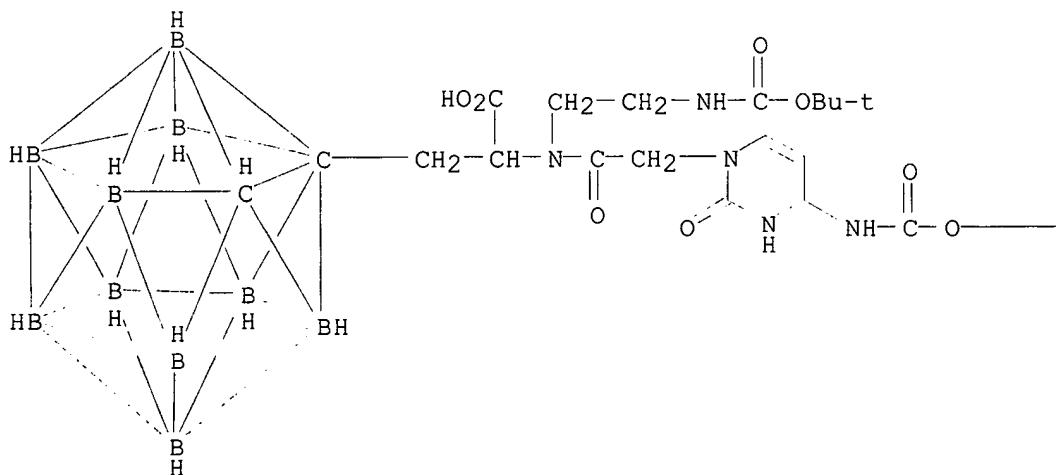


PAGE 1-B

— CH₂ — Ph

RN 288582-11-6 HCPLUS
 CN 1,2-Dicarbadodecaborane(12)-1-propanoic acid, .alpha.-[[[3,4-dihydro-2-oxo-4-[(phenylmethoxy)carbonyl]amino]-1(2H)-pyrimidinyl]acetyl][2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]amino]- (9CI) (CA INDEX NAME)

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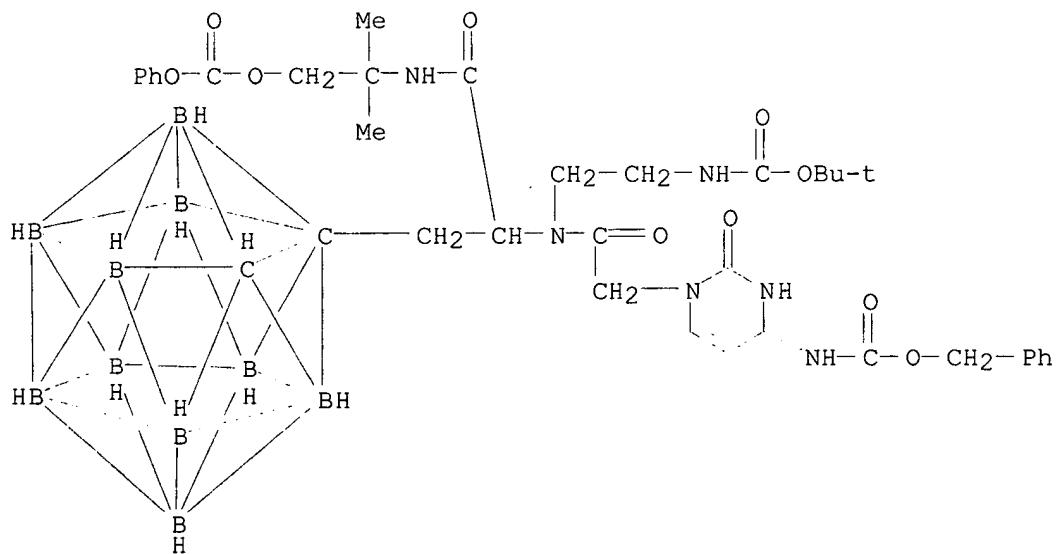


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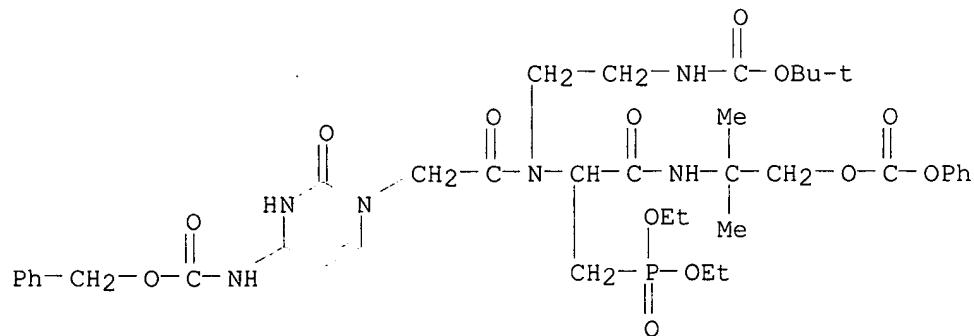
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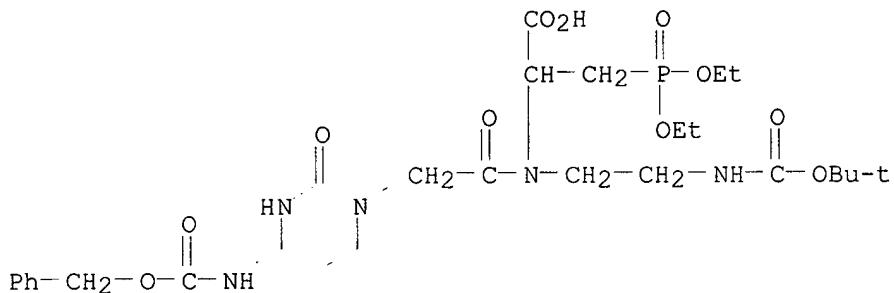
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CN 2-Oxa-5,8,11-triazadodecanedioic acid, 7-[(diethoxyphosphoryl)methyl]-8-[3,4-dihydro-2-oxo-4-[(phenylmethoxy)carbonyl]amino]-1(2H)-pyrimidinyl]acetyl]-4,4-dimethyl-6-oxo-, 12-(1,1-dimethylethyl) 1-phenyl ester (9CI) (CA INDEX NAME)



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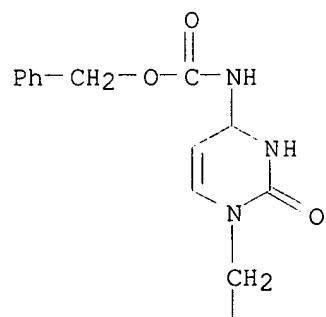
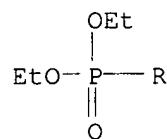
CN 9-Oxa-2,5-diaza-8-phosphaundecanoic acid, 6-carboxy-5-[[3,4-dihydro-2-oxo-4-[(phenylmethoxy)carbonyl]amino]-1(2H)-pyrimidinyl]acetyl]-8-ethoxy-, 1-(1,1-dimethylethyl) ester, 8-oxide (9CI) (CA INDEX NAME)



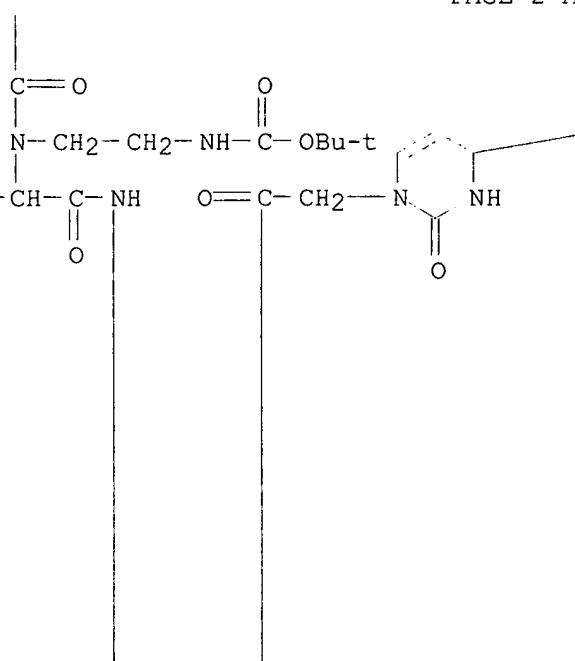
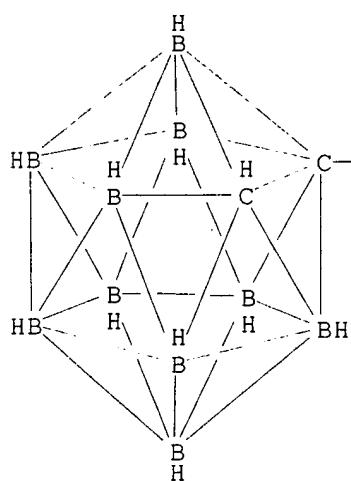
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CN 2,5,8,11,14,17-Hexaazanonadecanedioic acid, 6,18-bis(1,2-dicarbadodecaboran(12)-1-ylmethyl)-12-[(diethoxyphosphinyl)methyl]-5,11,17-tris[[3,4-dihydro-2-oxo-4-[(phenylmethoxy)carbonyl]amino]-1(2H)-pyrimidinyl]acetyl]-7,13-dioxo-, 1-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

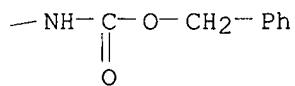
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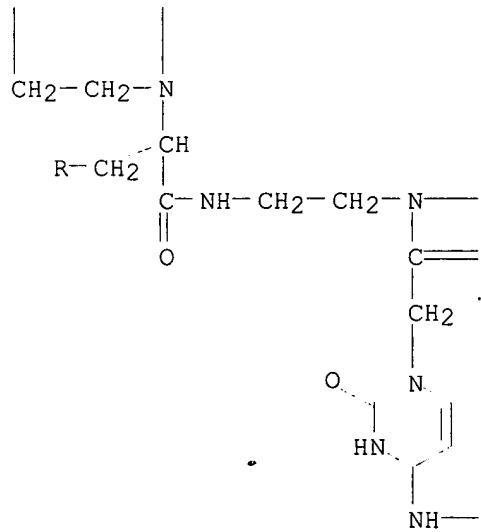
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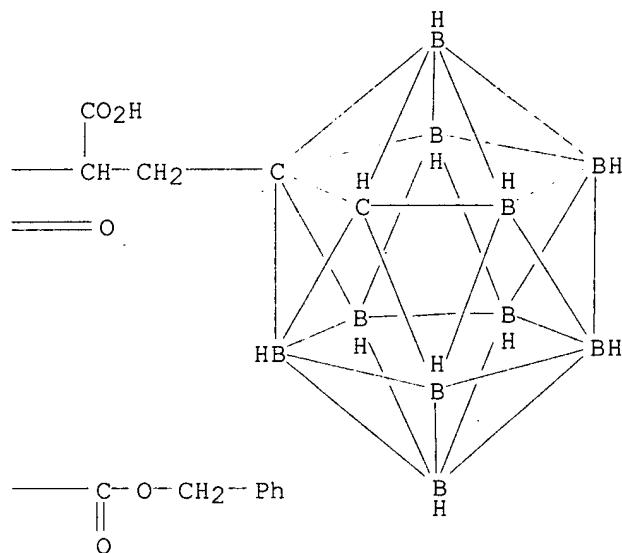
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PAGE 3-A



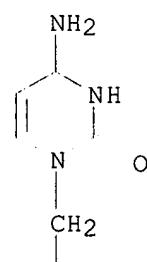
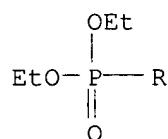
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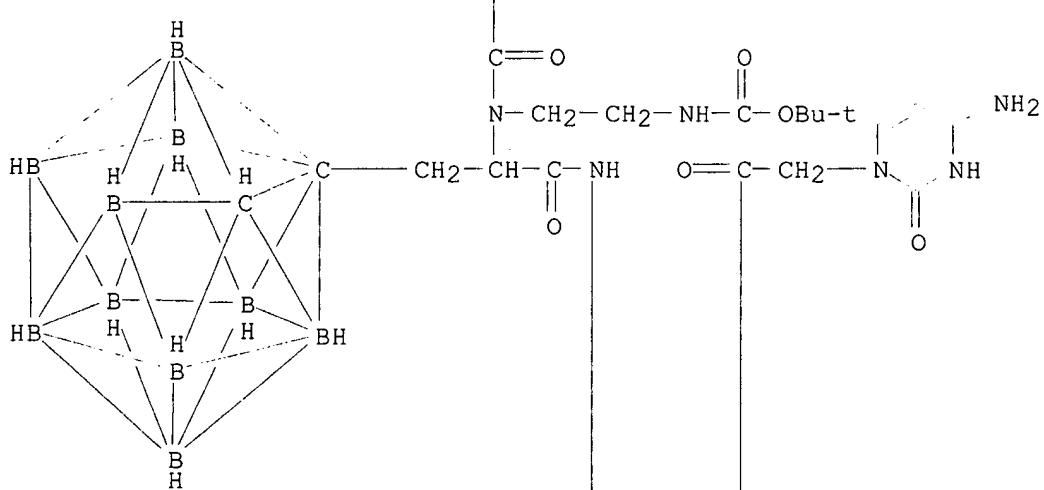
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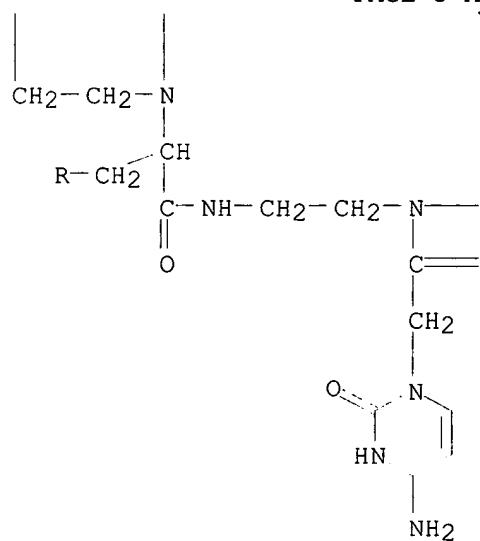
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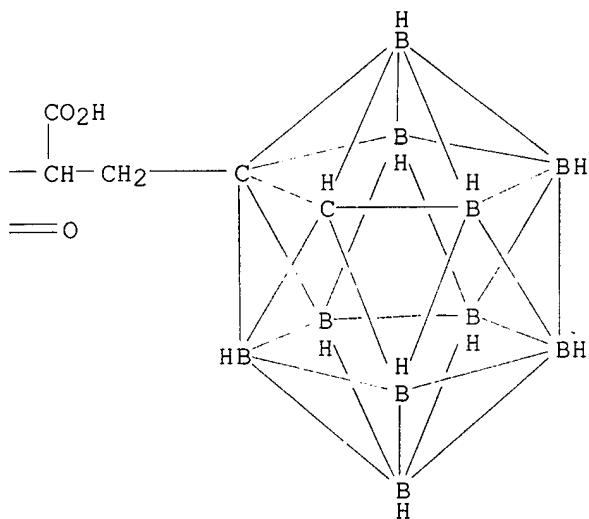
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PAGE 3-A



PAGE 3-B

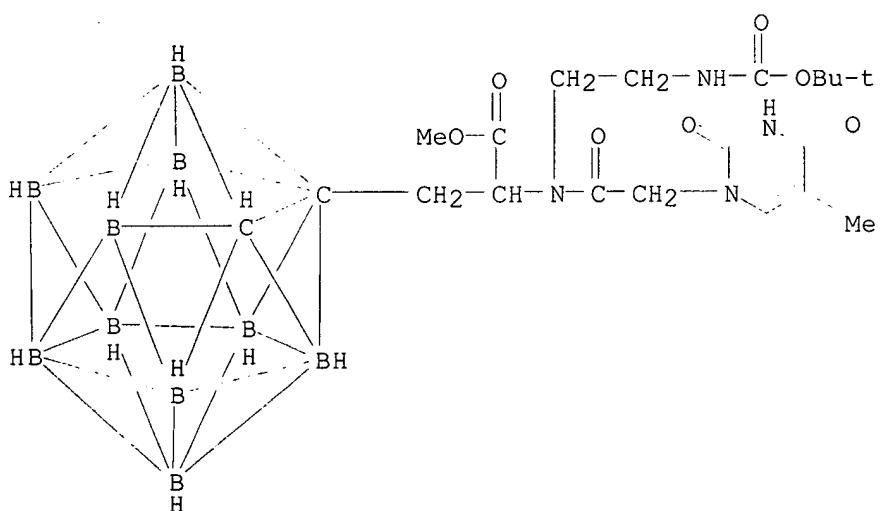


IT 288582-08-1P 288582-16-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of substituted monomers for synthesis of PNAs contg.
 carborane side-chains for use in cancer therapy)

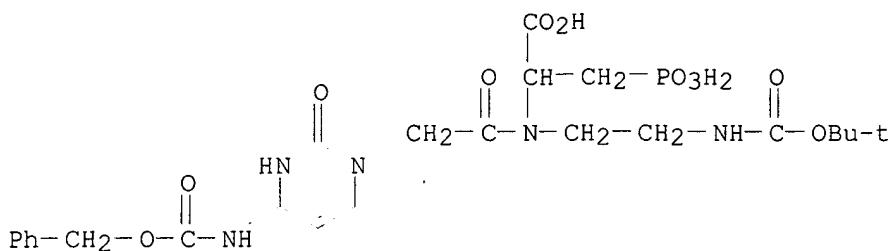
RN 288582-08-1 HCAPLUS

CN 1,2-Dicarbadodecaborane(12)-1-propanoic acid, .alpha.-[[3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl]acetyl][2-[[1,1-dimethylethoxy]carbonyl]amino]ethyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 288582-16-1 HCAPLUS

CN Alanine, N-[[3,4-dihydro-2-oxo-4-[(phenylmethoxy)carbonyl]amino]-1(2H)-pyrimidinyl]acetyl]-N-[2-[[1,1-dimethylethoxy]carbonyl]amino]ethyl]-3-phosphono- (9CI) (CA INDEX NAME)



L83 ANSWER 2 OF 5 HCPLUS COPYRIGHT 2003 ACS

AN 1997:155119 HCAPLUS

DN 126:165787

TI Preparation of gadolinium-DTPA complex containing a dicarbadodecaborane unit and intermediates thereof

IN Yamamoto, Yoshinori; Nemoto, Hisao

PA President of Tohoku University, Japan

SO Eur. Pat. Appl., 18 pp.

CODEN: EPXXDW

DT Patent

LA English

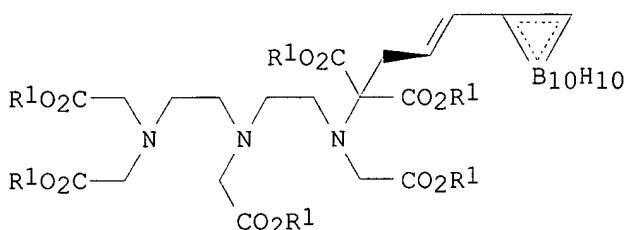
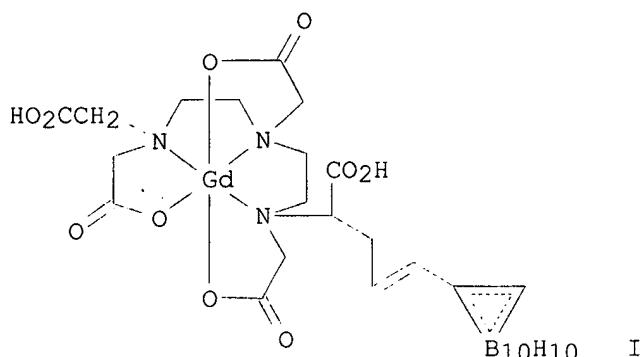
IC ICM C07F005-02

ICS C07E005-00

CC 78-7 (Inorganic Chemicals and Reactions)

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE | |
|------|-------------------|------|----------|-----------------|----------|--|
| PI | EP 754690 | A1 | 19970122 | EP 1996-111615 | 19960718 | |
| | EP 754690 | B1 | 20020213 | | | |
| | R: CH, DE, LI | | | | | |
| | JP 09031078 | A2 | 19970204 | JP 1995-185307 | 19950721 | |
| | US 5714591 | A | 19980203 | US 1996-682004 | 19960716 | |
| | AU 9660574 | A1 | 19970130 | AU 1996-60574 | 19960719 | |
| | AU 686951 | B2 | 19980212 | | | |
| PRAI | JP 1995-185307 | A | 19950721 | | | |
| OS | MARPAT 126:165787 | | | | | |
| GI | | | | | | |



AB The present invention provides Gd-diethylenetriaminepentaacetic acid (DTPA) complex I contg. a dicarbadodecaborane unit and intermediates thereof, i.e., carborane-contg. DTPA deriv. II (R1 = H or lower alkyl). The present invention also provides a method of synthesizing compd. I, which comprises reacting an ester deriv. of DTPA with a (1-carboxy-2-propenyl)dicarbadodecaborane deriv. in the presence of a Pd catalyst and an org. phosphine, e.g. [Pd(dbu)2] and dppe, deesterifying by treatment with an acid, reacting with GdCl3·6H2O, and treating with an alkali to give the desired compd. I. Complex I may be effective as a medicine relating to MRI and as a neutron capture agent used in radiotherapy of cancers (no data, use not in claims).

ST gadolinium DTPA dicarbadodecaboranyl prepn; diethylenetriaminepentaacetic acid dicarbadodecaboranyl gadolinium prepn; carborane diethylenetriaminepentaacetate gadolinium complex prepn

IT 32005-36-0, Bis(dibenzylideneacetone)palladium 52522-40-4
RL: CAT (Catalyst use); USES (Uses)
(catalyst with org. phosphine for prepn. of diethylenetriaminepentaacetate contg. dicarbadodecaborane unit)

IT 603-35-0, Triphenylphosphine, uses 824-11-3, Trimethylolpropane phosphite 1663-45-2, 1,2-Bis(diphenylphosphino)ethane .
RL: CAT (Catalyst use); USES (Uses)
(catalyst with palladium complex for prepn. of diethylenetriaminepentaacetate contg. dicarbadodecaborane unit)

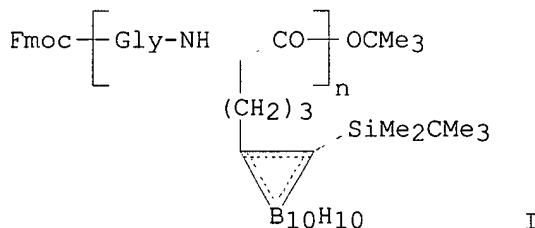
IT 67-43-6 541-41-3, Ethyl chloroformate 543-27-1, Isobutyl chloroformate 13450-84-5, Gadolinium chloride (GdCl3) hexahydrate 174472-54-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(for prepn. of gadolinium-diethylenetriaminepentaacetic acid complex contg. dicarbadodecaborane unit)

IT 51992-77-9P 174472-50-5P 174472-52-7P 174472-53-8P 174472-55-0P 186753-84-4P 186753-85-5P 186753-86-6P 186753-87-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for prepn. of gadolinium-diethylenetriaminepentaacetic acid complex contg. dicarbadodecaborane unit)

IT 174472-56-1P
RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of gadolinium-diethylenetriaminepentaacetic acid complex contg. dicarbadodecaborane unit)

L83 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2003 ACS
 AN 1993:192250 HCAPLUS
 DN 118:192250
 TI Solution-phase segment synthesis of boron-rich peptides
 AU Kane, Robert R.; Pak, Roger H.; Hawthorne, M. Frederick
 CS Dep. Chem. Biochem., Univ. California, Los Angeles, CA, 90024-1569, USA
 SO Journal of Organic Chemistry (1993), 58(5), 991-2
 CODEN: JOCEAH; ISSN: 0022-3263
 DT Journal
 LA English
 CC 34-3 (Amino Acids, Peptides, and Proteins)
 Section cross-reference(s): 8, 29
 OS CASREACT 118:192250
 GI



AB Small peptides I (Fmoc = 9-fluorenylmethoxycarbonyl; n = 1, 2, 4), contg. up to 40 boron atoms, were efficiently synthesized in soln. Condensation of a closo-carborane amino ester with Fmoc-Gly-F afforded the orthogonally protected dipeptide I (n = 1) in good yield. Selective removal of protecting groups allowed segment condensations, culminating with prodn. of the octapeptide I (n = 4). The lipophilic closo-carboranes in these peptides could be readily converted to their hydrophilic anionic nido derivs. This methodol. should find utility in the precise synthesis of boron-rich macromols., and should be esp. suited for use in the antibody mediated boron neutron capture therapy of cancer.

ST boron rich octapeptide; neutron capture therapy boron peptide; carborane peptide neutron capture therapy

IT Peptides, preparation
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (carborane-contg., prepn. of, as agents for neutron capture therapy)

IT Radiotherapy
 (neutron capture, prepn. of carborane-contg.
 peptides as agents for)

IT 81477-94-3, tert-Butyl N-(diphenylmethyleneglycinate
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (deprotonation and alkylation of, with (carboranyl)propyl iodides)

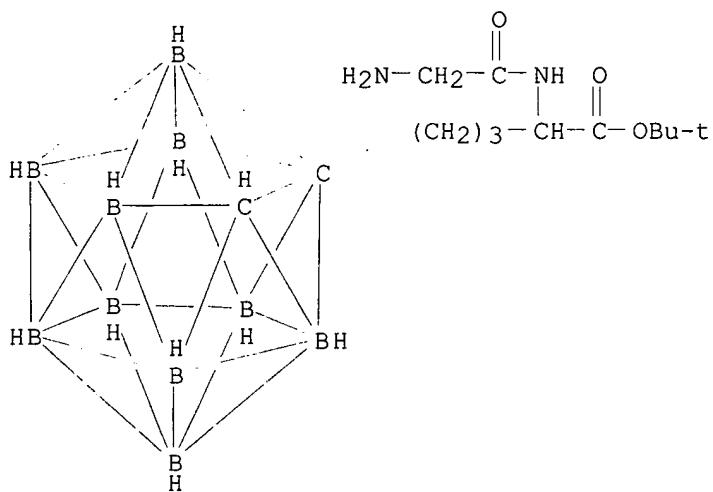
IT 130858-91-2, N-9-Fluorenylmethoxycarbonylglycyl fluoride
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (peptide coupling of, with carboranyl amino ester)

IT 146895-46-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and acidic hydrolysis of, carborane amino ester from)

IT 146912-77-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and conversion of, to anionic nido deriv.)

IT 146701-11-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
IT 146895-51-4P (prepn. and deblocking of, carboranyl octapeptide from)
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
IT 146895-54-7P (prepn. and peptide coupling of, with carboranyl dipeptide deriv.)
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
IT 146895-55-8P (prepn. and peptide coupling of, with carboranyl tetrapeptide deriv.)
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
IT 146895-48-9P (prepn. and peptide coupling of, with carboranyl tetrapeptide ester)
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
IT 146895-47-8P (prepn. and peptide coupling of, with protected glycyl fluoride)
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and substitution of, with (diphenylmethylene)glycinate enolate)
IT 146895-45-6P (prepn. and substitution of, with iodide)
IT 146665-27-2P 146665-29-4P 146701-10-2P 146895-49-0P (prepn. of)
RL: SPN (Synthetic preparation); PREP (Preparation)
IT 146895-50-3P 146895-53-6P (prepn. (prepn., deblocking, or deesterification of))
RL: SPN (Synthetic preparation); PREP (Preparation)
IT 146895-52-5P (prepn. (prepn., desilylation, or peptide coupling of, with carboranyl
dipeptide ester))
IT 12586-31-1 (RCT (Reactant); RACT (Reactant or reagent))
(radiotherapy, neutron capture, prepn. of carborane-contg. peptides as
agents for)
IT 23868-53-3 (PROC (Process))
(substitution of, with (diphenylmethylene)glycinate enolate)
IT 138490-27-4 (RCT (Reactant); RACT (Reactant or reagent))
(tosylation of, or Mitsunobu substitution of, with iodide)
IT 146912-77-8P (SPN (Synthetic preparation); PREP (Preparation))
(prepn. and conversion of, to anionic nido deriv.)
RN 146912-77-8 HCPLUS
CN Norleucine, 5-(1,2-dicarbadodecaboran(12)-1-yl)-N-glycyl-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

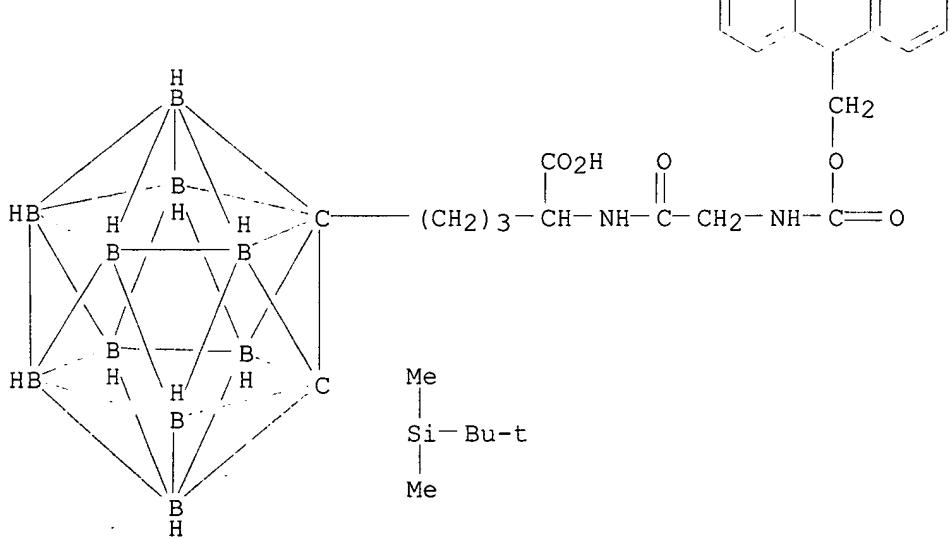


IT 146895-51-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and peptide coupling of, with carboranyl dipeptide deriv.)

RN 146895-51-4 HCAPLUS

CN Norvaline, 5-[2-[(1,1-dimethylethyl)dimethylsilyl]-1,2-dicarbadodecaboran(12)-1-yl]-N-[N-[(9H-fluoren-9-ylmethoxy)carbonyl]glycyl]- (9CI) (CA INDEX NAME)



IT 146895-54-7P

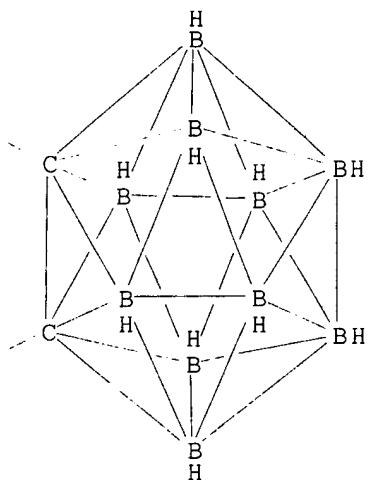
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and peptide)

RN 146895-54-7 HCPLUS
CN Norvaline, glycyl-5-[2-[(1,1-dimethylethyl)dimethylsilyl]-1,2-dicarbadodecaboran(12)-1-yl]norvalylglycyl-5-[2-[(1,1-dimethylethyl)dimethylsilyl]-1,2-dicarbadodecaboran(12)-1-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 1-B



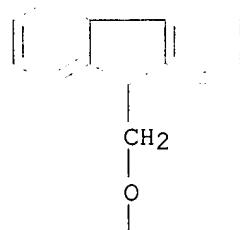
IT 146895-55-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and peptide coupling of, with carboranyl tetrapeptide ester)

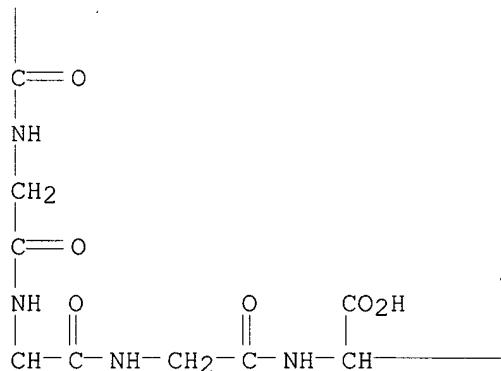
RN 146895-55-8 HCPLUS

CN Norvaline, N-[(9H-fluoren-9-ylmethoxy)carbonyl]glycyl-5-[2-[(1,1-dimethylethyl)dimethylsilyl]-1,2-dicarbadodecaboran(12)-1-yl]norvalylglycyl-5-[2-[(1,1-dimethylethyl)dimethylsilyl]-1,2-dicarbadodecaboran(12)-1-yl]-(9CI) (CA INDEX NAME)

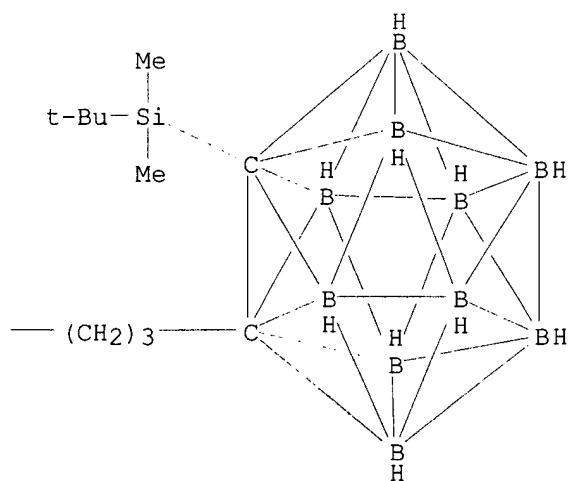
PAGE 1-A



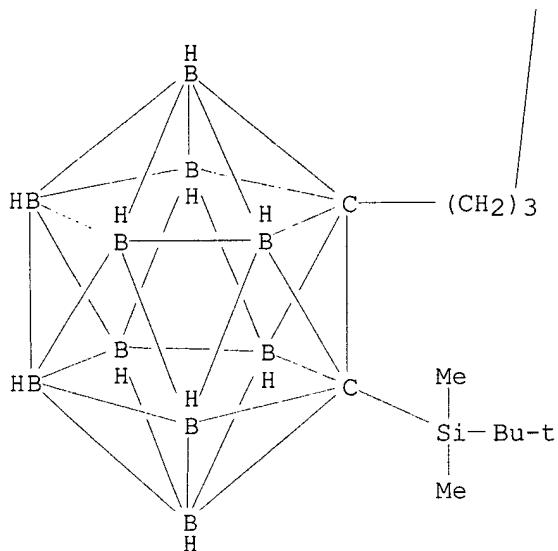
PAGE 2-A



PAGE 2-B



PAGE 3-A



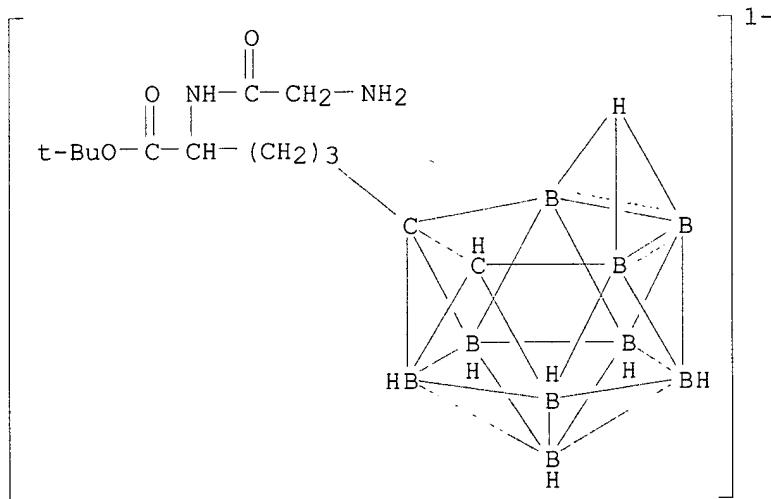
IT 146665-27-2P 146665-29-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 146665-27-2 HCAPLUS

CN 7,8-Dicarbaundecaborate(1-), 7-[4-[(aminoacetyl)amino]-5-(1,1-dimethylethoxy)-5-oxopentyl]undecahydro-, sodium (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

 Na^+

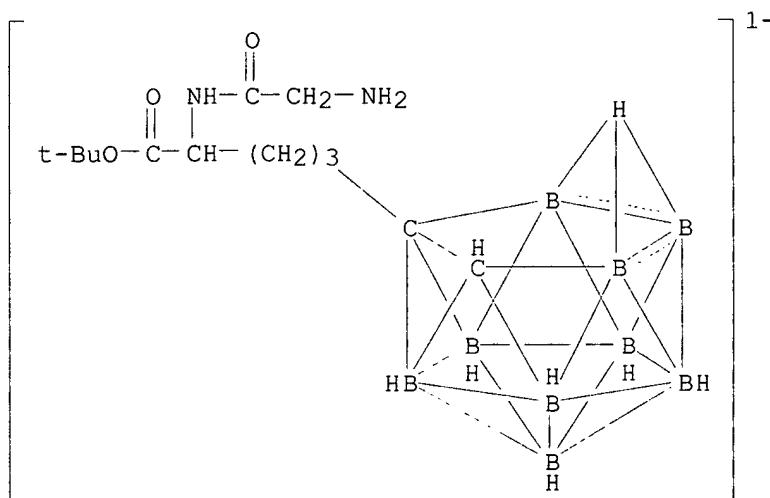
RN 146665-29-4 HCAPLUS

CN 7,8-Dicarbaundecaborate(1-), 7-[4-[(aminoacetyl)amino]-5-(1,1-dimethylethoxy)-5-oxopentyl]undecahydro-, hydrogen, compd. with pyrrolidine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 146665-28-3
 CMF C13 H32 B9 N2 O3 . H

PAGE 1-A



PAGE 2-A

● H⁺

CM 2

CRN 123-75-1
 CMF C4 H9 N

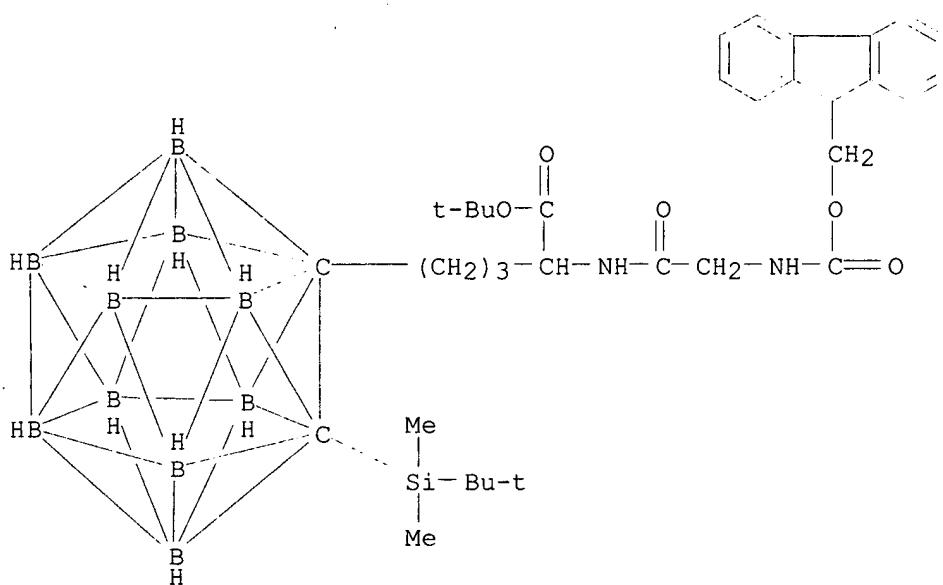


IT 146895-50-3P 146895-53-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn., deblocking, or deesterification of)

RN 146895-50-3 HCPLUS

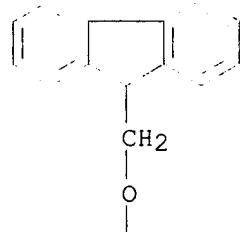
CN Norvaline, 5-[2-[(1,1-dimethylethyl)dimethylsilyl]-1,2-dicarbadodecaboran(12)-1-yl]-N-[N-[(9H-fluoren-9-ylmethoxy)carbonyl]glycyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



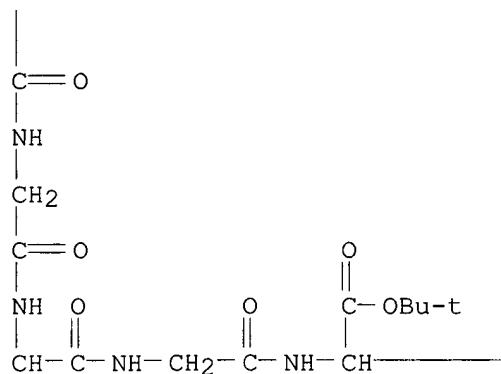
RN 146895-53-6 HCAPLUS

CN Norvaline, N-[(9H-fluoren-9-ylmethoxy)carbonyl]glycyl-5-[2-[(1,1-dimethylethyl)dimethylsilyl]-1,2-dicarbadodecaboran(12)-1-yl]norvalylglycyl-5-[2-[(1,1-dimethylethyl)dimethylsilyl]-1,2-dicarbadodecaboran(12)-1-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

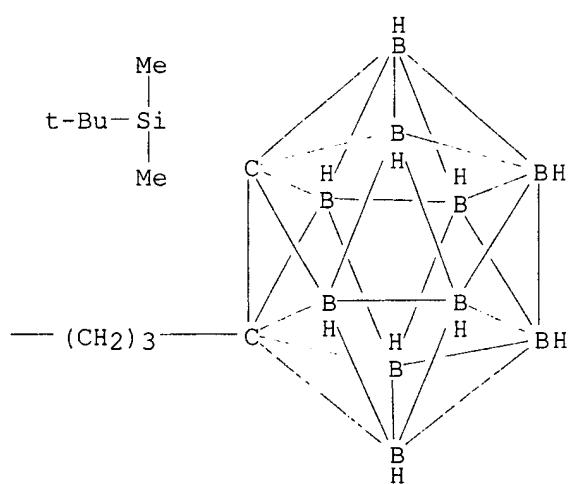
PAGE 1-A



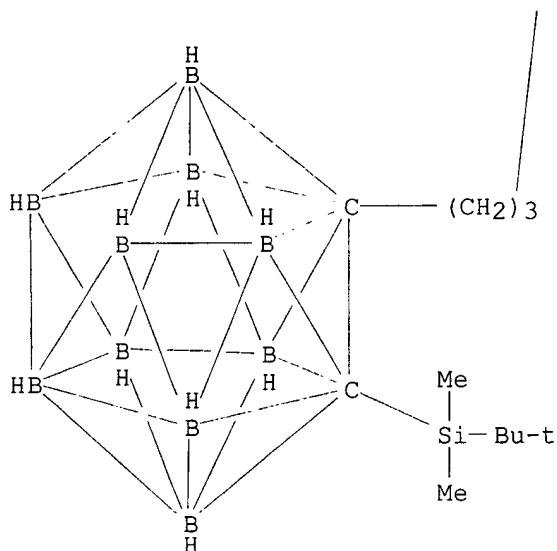
PAGE 2-A



PAGE 2-B



PAGE 3-A

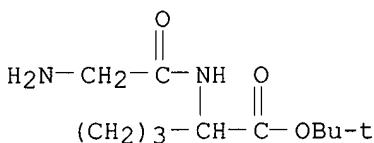
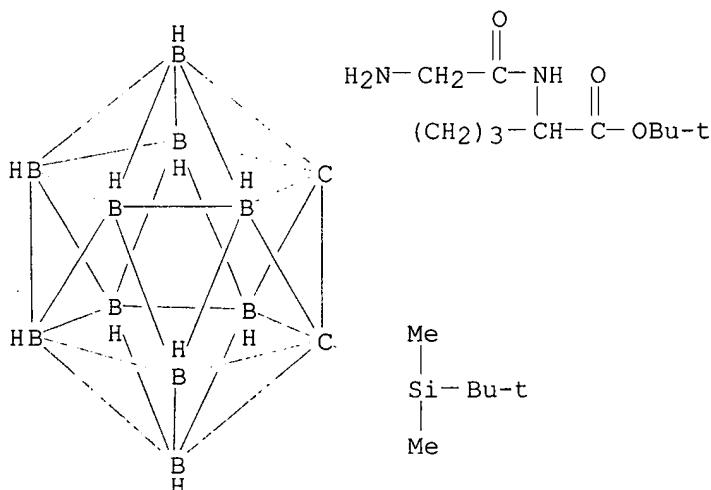


IT 146895-52-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., desilylation, or peptide coupling of, with carboranyl dipeptide ester)

RN 146895-52-5 HCPLUS

CN Norvaline, 5-[2-[(1,1-dimethylethyl)dimethylsilyl]-1,2-dicarbadodecaron(12)-1-yl]-N-glycyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L83 ANSWER 4 OF 5 HCPLUS COPYRIGHT 2003 ACS

AN 1992:251163 HCPLUS

DN 116:251163

TI Carboranyl peptide-antibody conjugates for neutron-capture therapy: preparation, characterization, and in vivo evaluation

AU Paxton, Raymond J.; Beatty, Barbara G.; Varadarajan, Aravamuthan; Hawthorne, M. Frederick

CS Div. Immunol., Beckman Res. Inst. City of Hope, Duarte, CA, 91010, USA

SO Bioconjugate Chemistry (1992), 3(3), 241-7
CODEN: BCCHES; ISSN: 1043-1802

DT Journal

LA English

CC 8-9 (Radiation Biochemistry)

Section cross-reference(s): 15

AB Two model peptides rich in boron and prep'd. by Merrifield syntheses, dansyl.(nido-CB)2 (I) and dansyl.(nido-CB)10.Lys.Ac (II), where nido-CB represents the .alpha.-amino acid [nido-7-CH3-8-(CH2)3CH(NH2)COOH-C2B9H]- were conjugated with the anti-CEA mAb T84.66 using peptide active ester reagents. The dansyl groups provided a means of fluorometric anal. of mAb conjugates which was augmented by conventional amino acid analyses for nido-CB. The conjugate of I contained an av. of 63 B atoms per mAb mol. The mAb conjugate of II was chromatog. sepd. into a strongly fluorescent high-mol.-wt. aggregated fraction (HMW) and a less intensely fluorescent monomeric fraction. Both fractions retained immunoreactivity. The HMW species contained an av. of .apprx.490 B atoms/mAb mol., as detd. by amino acid anal. Biodistribution data were collected using nude mice bearing LS174T xenografts and 125I-labeled mAb conjugates. While the lightly B-loaded dipeptide conjugate gave biodistribution results which resembled those of native T84.66 mAb, the undecapeptide conjugate displayed greatly enhanced liver uptake and decreased tumor accretion. As the boron-contg. burden on the supporting immunoprotein is greatly increased, as in the case of the T84.66-II conjugate, loss of circulating conjugate to liver effectively competes with the desired tumor localization. Means which might be taken to circumvent this difficulty have been previously described.

ST carboranyl peptide monoclonal antibody conjugate prepn; boron neutron capture radiotherapy carboranyl peptide

IT Antigens
RL: SPN (Synthetic preparation); PREP (Preparation)
(CEA (carcinoembryonic antigen), monoclonal antibodies to, carboranyl peptide conjugates, prepn. and biodistribution of, in neoplasia, boron-neutron-capture radiotherapy in relation to)

IT Immunoglobulins
RL: SPN (Synthetic preparation); PREP (Preparation)
(G1, monoclonal, conjugates, with carboranyl peptides, prepn. and biodistribution of, in neoplasm, boron-neutron capture radiotherapy in relation to)

IT Radiotherapy
(boron-neutron capture, of neoplasms, carboranyl peptide-monoclonal antibody conjugates prepn. for)

IT Antibodies
RL: SPN (Synthetic preparation); PREP (Preparation)
(monoclonal, conjugates, carboranyl peptide, to carcinoembryonic antigens, prepn. and biodistribution of, in neoplasia, boron-neutron capture radiotherapy in relation to)

IT 134815-43-3DP, anti-carcinoembryonic antigen monoclonal antibody conjugates 135105-48-5DP, anti-carcinoembryonic antigen monoclonal antibody conjugates
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(prepn. and biodistribution of, in tumor, boron-neutron capture radiotherapy in relation to)

IT 12586-31-1
RL: BIOL (Biological study)
(radiotherapy, boron-neutron capture, of neoplasms, carboranyl peptide-monoclonal antibody conjugates prepn. for)

IT 134815-43-3DP, anti-carcinoembryonic antigen monoclonal antibody conjugates
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); OCCU (Occurrence); PREP

(Preparation)

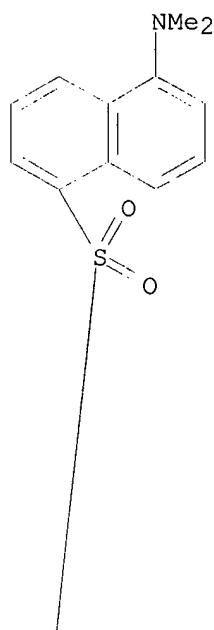
(prepn. and biodistribution of, in tumor, boron-neutron capture
radiotherapy in relation to)

RN 134815-43-3 HCPLUS

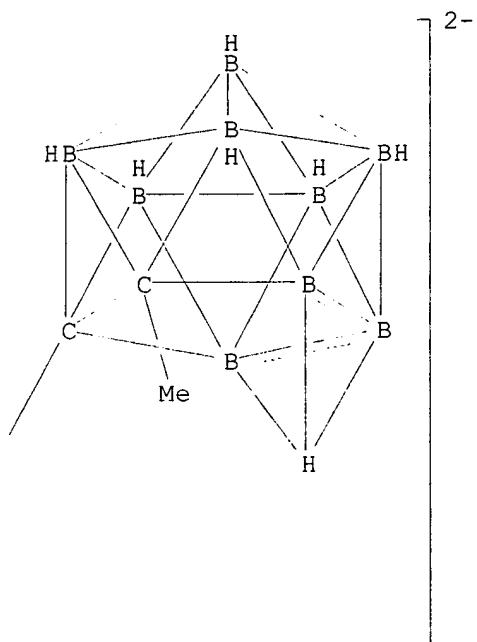
CN 7,8-Dicarbaundecaborate(3-), 7,7'-.mu.-[(4-carboxylato-1,4-
butanediyl)imino[2-[[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]amino]-1-
oxo-1,5-pentanediy]]eicosahydro-8,8'-dimethylbis-, disodium hydrogen,
[S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

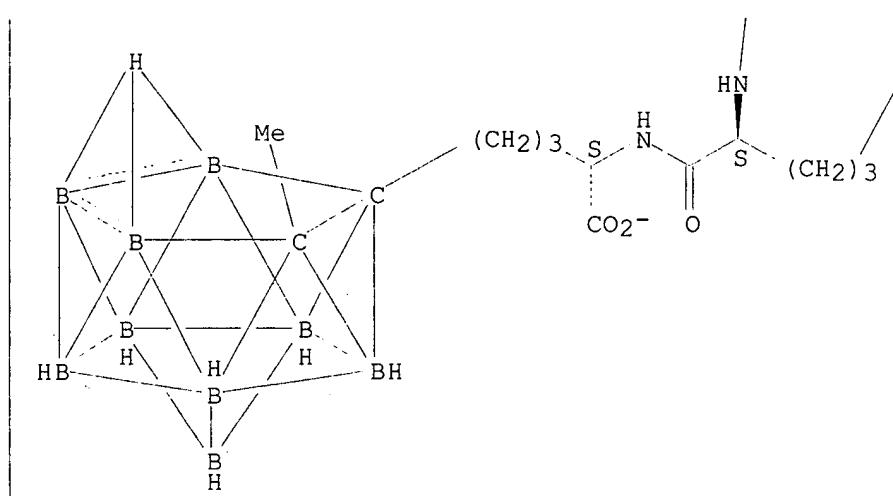
PAGE 1-A



PAGE 1-B



PAGE 2-A

● H^+

PAGE 2-B

●2 Na⁺

L83 ANSWER 5 OF 5 HCPLUS COPYRIGHT 2003 ACS
AN 1991:492903 HCPLUS
DN 115:92903
TI Novel carboranyl amino acids and peptides: reagents for antibody modification and subsequent neutron-capture studies
AU Varadarajan, Aravamuthan; Hawthorne, M. Frederick
CS Dep. Chem. Biochem., Univ. California, Los Angeles, CA, 90024, USA
SO Bioconjugate Chemistry (1991), 2(4), 242-53
CODEN: BCCHES; ISSN: 1043-1802
DT Journal
LA English
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 9, 29
AB A new alpha.-amino acid deriv. incorporating the 1,2-dicarba-closo-dodecarborane(12) cage H₂NCH(CH₂CH₂CH₂R)CO₂H [I; R = 2-methyl-1,2-dicarba-closo-dodecaborane(12)-1-yl] was prep'd. by alkylation of Ph₂C:NCH₂CO₂Me with 3-(2-methyl-1,2-dicarba-closo-dodecaborane(12)-1-yl)propyl iodide. I was employed in the synthesis of peptide derivs. such as R₁-[NHCH(CH₂CH₂CH₂R)CO]₂-OH (II; R₁ = H) and R₁-[NHCH(CH₂CH₂CH₂R)CO]_n-Lys-OH (III; R₁ = H; n = 5, 10) (IV) using solid-phase Merrifield methods. Dipeptide II (R₁ = H) was converted to a water-sol. ionic deriv. by the pyrrolidine-mediated carborane cage degrdn. reaction followed by cation exchange to afford the sodium salt II [R = 2-methyl-1,2-dicarba-nido-undecaborane(12)-1-yl sodium salt; R₁ = H]; dansylation with dansyl chloride yielded the fluorescence-labeled dipeptide II (R = same, R₁ = dansyl). Undecapeptide IV (n = 10) was dansylated while still anchored to the Merrifield resin. Following its cleavage from the resin with HF, the product was acetylated to block the free amino group on the lysine residue and then converted to the water-sol. deriv. III (R = same, R₁ = dansyl, n = 10). Trial conjugations of the nido dipeptide and undecapeptide to T84.66, an anti-CEA antibody, were carried out by of carboxyl activation with N-hydroxysulfosuccinimide and N,N-diisopropylcarbodiimide. Studies of the chem. syntheses of these and other peptide derivs. and the conjugation to the antibody are described.
ST carborane oligopeptide conjugate antibody; carboranyl amino acid peptide coupling; alkylation methyldicarbadodecaboranylpropyl iodide glycine Schiff base
IT Antibodies
RL: RCT (Reactant); RACT (Reactant or reagent)
(T-84.66, conjugation of, with dicarbododecaborane-contg.

oligopeptides)

IT Peptides, preparation
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (dicarbododecaborane-contg., prepn., conversion of, to anionic nido derivs., and conjugation of, with antibodies)

IT 81167-39-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (alkylation of, with (dicarbododecaborane)propyl iodide)

IT 82436-78-0, N-Hydroxysulfosuccinimide
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (conjugation by, of dicarbododecaborane-contg. **oligopeptides** with antibody T84.66)

IT 605-65-2, Dansyl chloride
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (dansylation by, of dicarbododecaborane-contg. **oligopeptides**)

IT 135105-47-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. and acetylation of)

IT 77653-10-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. and alkylation by, of glycine Schiff base)

IT 134781-34-3P 134815-42-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and attempted solid-phase peptide coupling reactions of)

IT 134815-43-3P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and conjugation of, to T84.66 antibody with hydroxysulfosuccinimide)

IT 134781-31-0P 135105-49-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and conversion of, to anionic nido deriv., with pyrrolidine)

IT 134815-44-4P 135105-45-2P 135105-46-3DP, resin-bound
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. and dansylation of)

IT 134781-27-4P 134781-28-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. and hydrolysis of)

IT 134781-30-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. and solid-phase peptide coupling reactions of)

IT 134781-26-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and substitution of, with sodium iodide)

IT 134815-43-3DP, conjugate with hydroxysulfosuccinimide and T84.66 antibody 135105-50-9P 135105-51-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

IT 108204-94-0P 134781-29-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn., butoxycarbonylation, and conversion of, to anionic nido deriv.)

IT 134781-32-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn., butoxycarbonylation, and salt exchange of)

IT 56-12-2, 4-Aminobutanoic acid, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (solid-phase peptide coupling reactions of, dicarbododecaborane-contg. **oligopeptide** from)

IT 4530-20-5 54613-99-9 57294-38-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (solid-phase peptide coupling reactions of, dicarbadodecaborane-contg.
 oligopeptides from)

IT 17815-32-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (tosylation of)

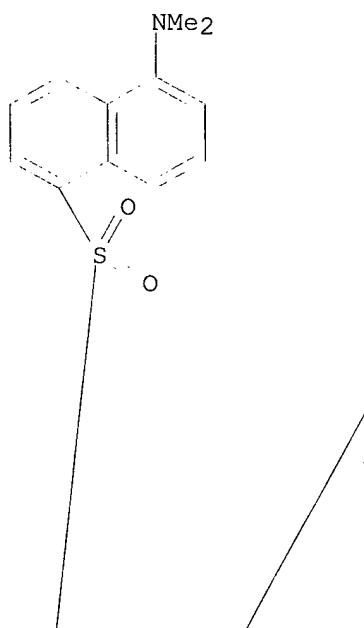
IT 134815-43-3P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and conjugation of, to T84.66 antibody with
 hydroxysulfosuccinimide)

RN 134815-43-3 HCPLUS

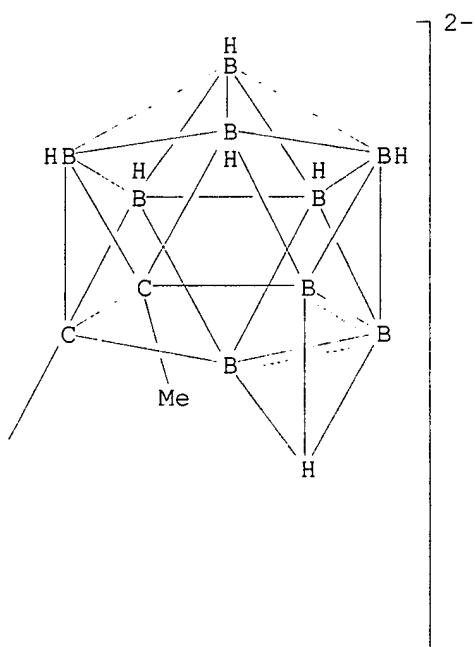
CN 7,8-Dicarbaundecaborate(3-), 7,7'-.mu.-[(4-carboxylato-1,4-
 butanediyl)imino[2-[[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]amino]-1-
 oxo-1,5-pentanediy]]]eicosahydro-8,8'-dimethylbis-, disodium hydrogen,
 [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

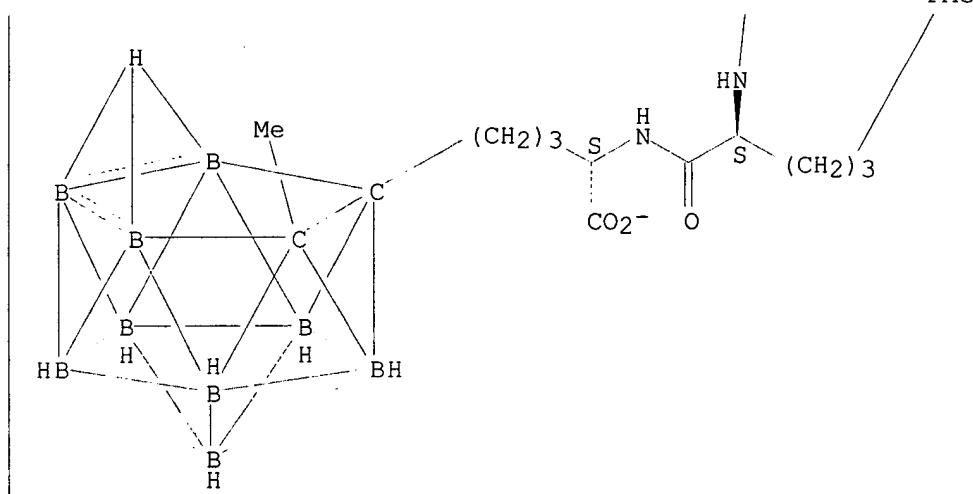
PAGE 1-A



PAGE 1-B



PAGE 2-A

 $\bullet H^+$

PAGE 2-B

●2 Na⁺

IT 134781-31-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conversion of, to anionic nido deriv., with pyrrolidine)

RN 134781-31-0 HCPLUS

CN 1,2-Dicarbadodecaborane(12)-1-pentanoic acid, a-[[2-amino-5-(2-methyl-1,2-dicarbadodecaboran(12)-1-yl)-1-oxopentyl]amino]-2-methyl-, [S-(R*,R*)]-
(9CI) (CA INDEX NAME)

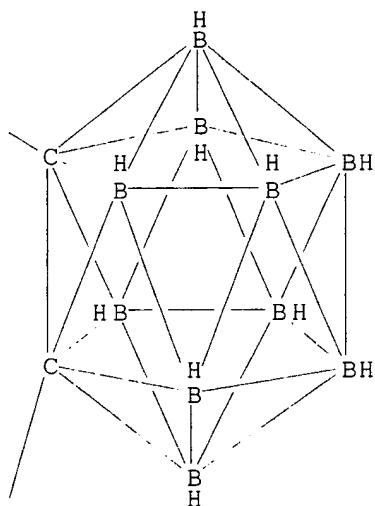
Absolute stereochemistry.

PAGE 1-A

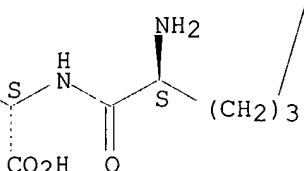
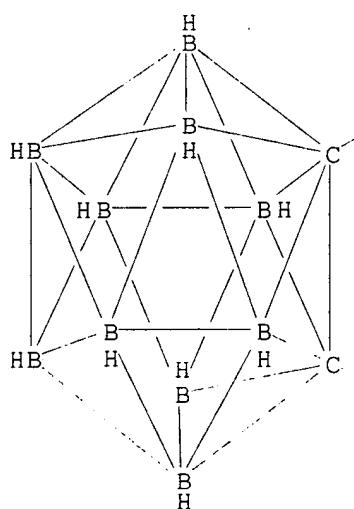
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PAGE 1-B



PAGE 2-A



IT 134815-44-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prep. and dansylation of)

RN 134815-44-4 HCAPLUS

CN 7,8-Dicarbaundecaborate(3-), 7,7'-.mu.-[(4-amino-5-oxo-1,5-pentanediyl)imino(1-carboxylato-1,4-butanediyl)]eicosahydro-8,8'-dimethylbis-, disodium hydrogen, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

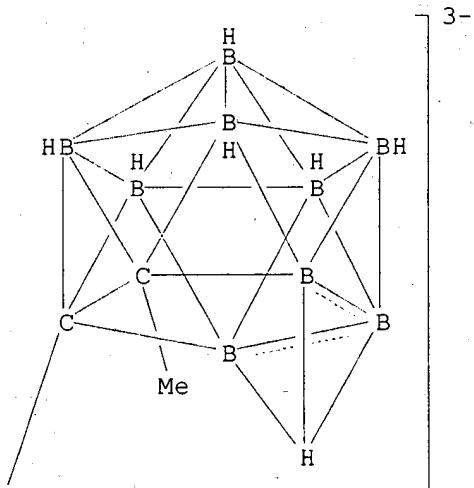
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Page 38

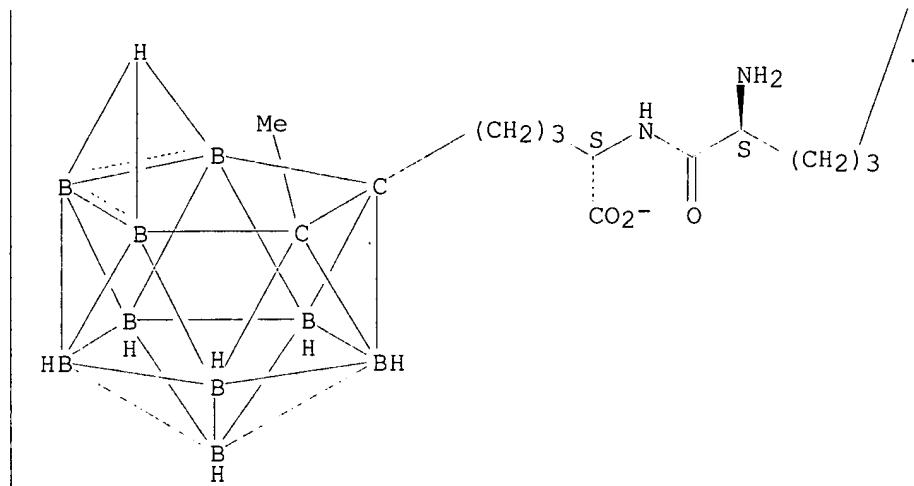
PAGE 1-A



PAGE 1-B



PAGE 2-A

● H^+

PAGE 2-B

● 2 Na^+

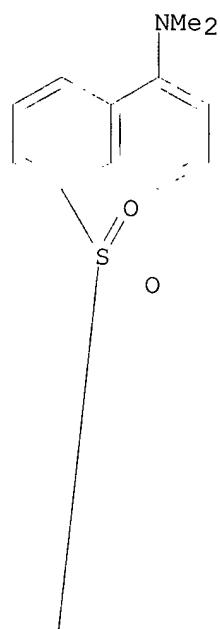
IT 134815-43-3DP, conjugate with hydroxysulfosuccinimide and T84.66 antibody
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 134815-43-3 HCPLUS

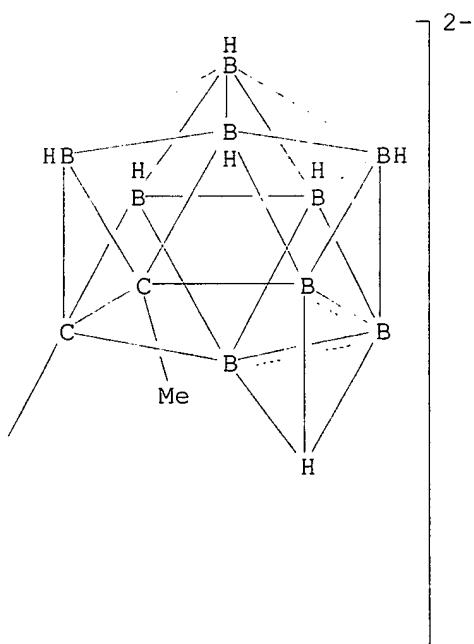
CN 7,8-Dicarbaundecaborate(3-), 7,7'-.mu.-[(4-carboxylato-1,4-butanediyi)imino{2-[[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]amino]-1-oxo-1,5-pentanediyi}]]eicosahydro-8,8'-dimethylbis-, disodium hydrogen, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

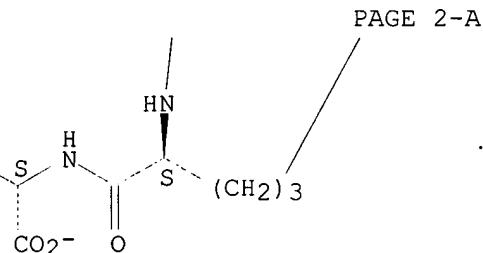
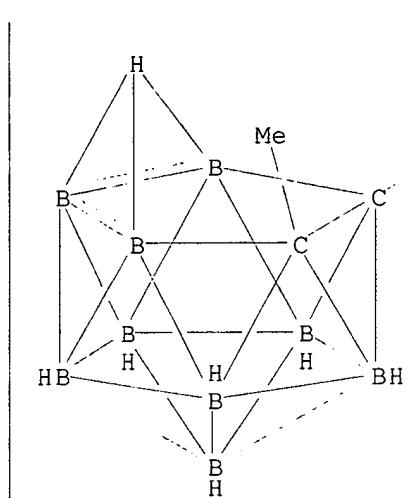
Absolute stereochemistry.

PAGE 1-A



PAGE 1-B





● H⁺

PAGE 2-B

● 2 Na⁺